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Sierra Mechanics Code Overview

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Sandia is a multi program laboratory operated by Sandia Corporation, a Lockheed Martin Company,
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The national code strategy establishes Sandia as the engineering simulation capability provider

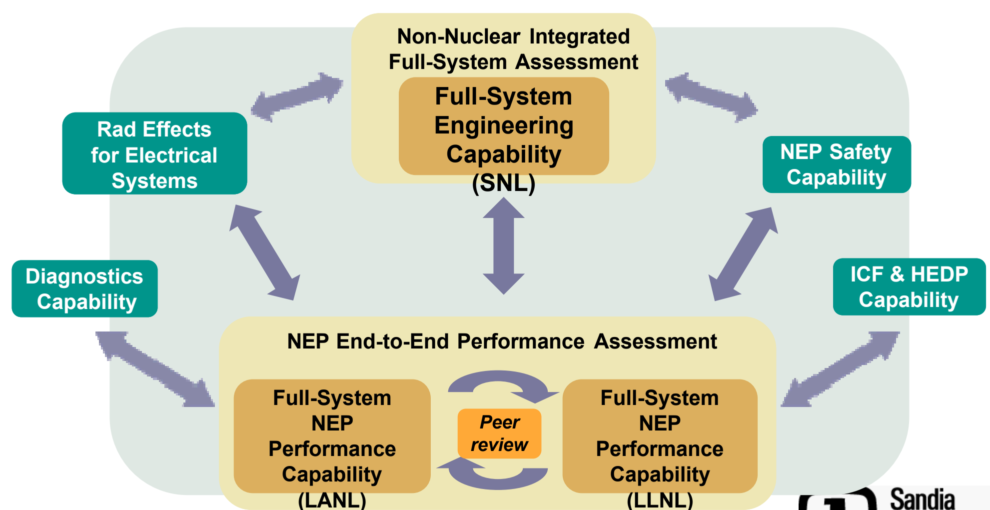
Focus Areas	Current State	Strategies	Future State
Integrated Simulation Capabilities (Application Codes)	• 14 modern + numerous legacy codes across 6 broad application areas • Core physics simulation competencies established	Establish the National Simulation Portfolio for Stockpile Certification	• 7 modern national capabilities • End legacy development • Core competencies sustained
Computational Science	• Tera scale computational science established (MPI programming model) • Basic capabilities for uncertainty quantification	Advance computational algorithms to enable predictive simulation and QMU	• Algorithms & programming models supporting predictive simulation at petaFLOP and exaFLOP scales • Advanced capabilities for uncertainty quantification and QMU studies
Scope of Applications	• ASC simulation capabilities focused on certification for tail numbers	Broaden the impact of ASC simulation capabilities in national security	• Capabilities for broader national security applications, including NNSA nuclear security and non-proliferation missions

Strategic Components

1. Establish the National Simulation Portfolio for Weapons Science and Engineering, and Stockpile Certification
   - *Define the core simulation capabilities needed*
   - *End development funding for legacy codes*
   - *Establish the capability to couple between codes of national portfolio*
2. Advance Computational Algorithms to Enable Predictive Simulation and QMU
   - *Advance scalability of computational algorithms*
   - *Collaborate on evolution of programming models*
   - *Deliver advanced capabilities for QMU and UQ*
3. Broaden the Impact of ASC Simulation Capabilities in National Security
   - *Develop a business "prospectus" for major capabilities*
   - *Develop and support interagency partnerships*
   - *Develop enhanced capabilities for expanded national security missions*

Objectives

1. ***Advance world-leading predictive science***, providing the capability to sustain stockpile stewardship without returning to underground nuclear testing as weapons age and we move further from the test base.
2. ***Enable Quantification of Margins and Uncertainties (QMU)-based certification***, transforming the broader certification process to allow more effective and selective use of aboveground experiment, certification tests, flight tests, and other tests.
3. ***Catalyze a responsive infrastructure*** through pervasive simulation across all aspects of the stockpile lifecycle, such as design, certification, manufacturing, Significant Finding Investigation resolution, transportation, security, safe dismantlement, outputs and environments, etc.
4. ***Enable a broadened national security mission***, in which simulation tools extend beyond stockpile stewardship and enable the next-generation mission of the Complex



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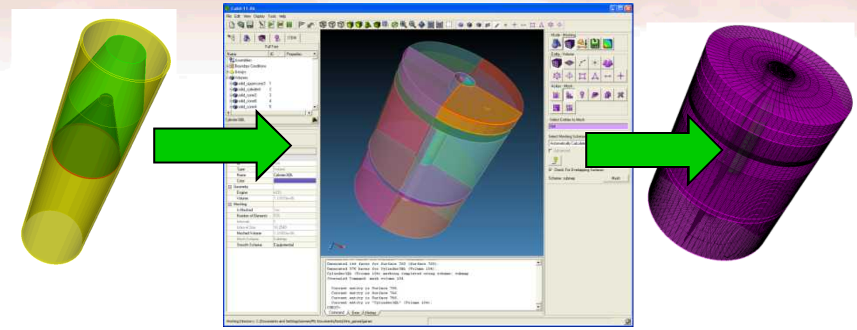
Geometry and Mesh Generation Toolkit



CAD Model

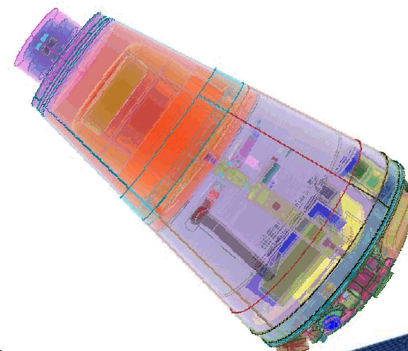
CUBIT

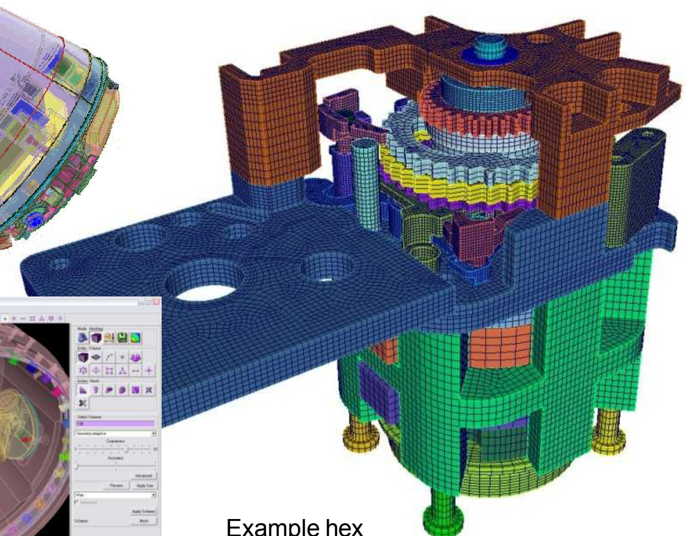
Mesh

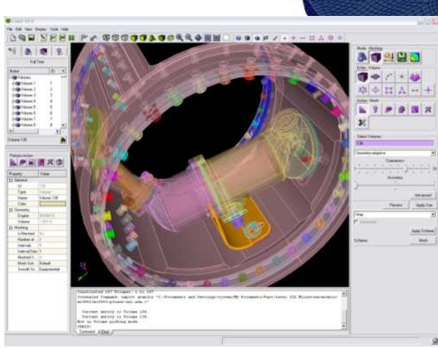
CUBIT accepts a CAD model as input, and exports a finite element mesh ready for analysis

CAD-Based Meshing Toolkit

- Specializes in all-hex meshes for complex assemblies
- CAD geometry diagnostics, clean-up and decomposition tools
- Automatic hex, tet, quad, tri meshing schemes
- Includes wizard-based workflow for model prep.
- Element quality diagnostics and mesh improvement
- Professional cross-platform GUI
- Command/script driven interface
- Supports multiple CAD and mesh formats







Example hex meshes generated with CUBIT

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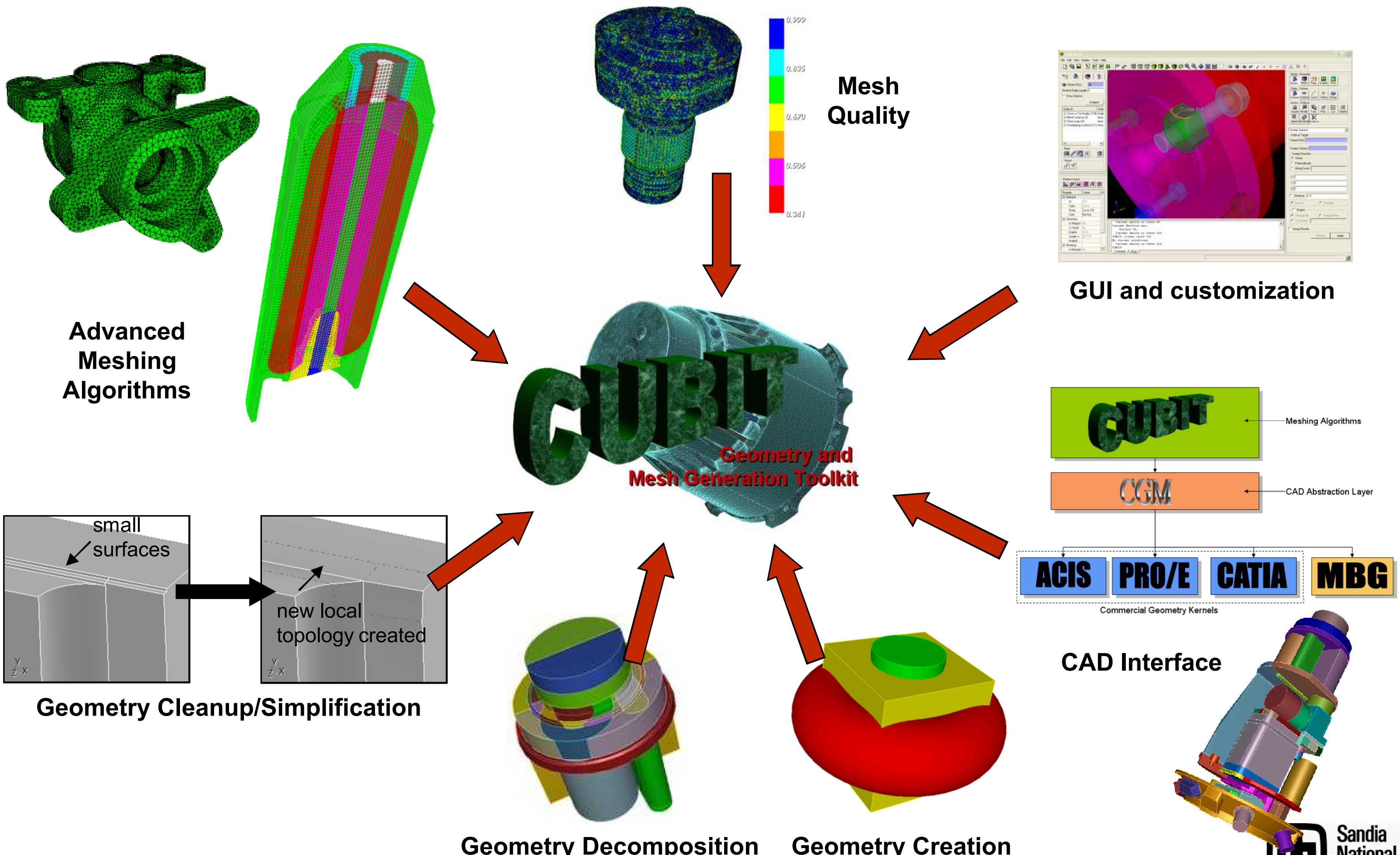
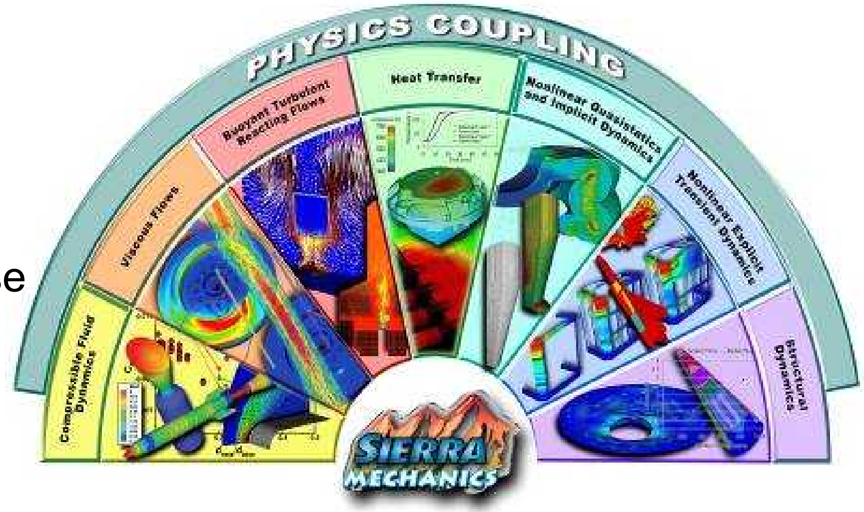
Capabilities



SIERRA has a wide range of coupled mechanics simulation capabilities

- **Thermal/fluids/aerodynamics**
  - Compressible fluid mechanics with subsonic through hypersonic flows
  - Non-newtonian reacting flow with free surfaces and complex material response
  - Low mach number turbulent reacting flow participating media radiation
  - Heat transfer with limited convection, chemistry, and enclosure radiation



- **Solid mechanics/structural dynamics**
  - Nonlinear solid mechanics, quasistatics, implicit dynamics, failure and tearing
  - Nonlinear solid dynamics with explicit time integration, nodal-based tets, remeshing, particle methods, cohesive surface elements, contact, and material failure
  - Linear structural dynamics and modal analysis of complex structures

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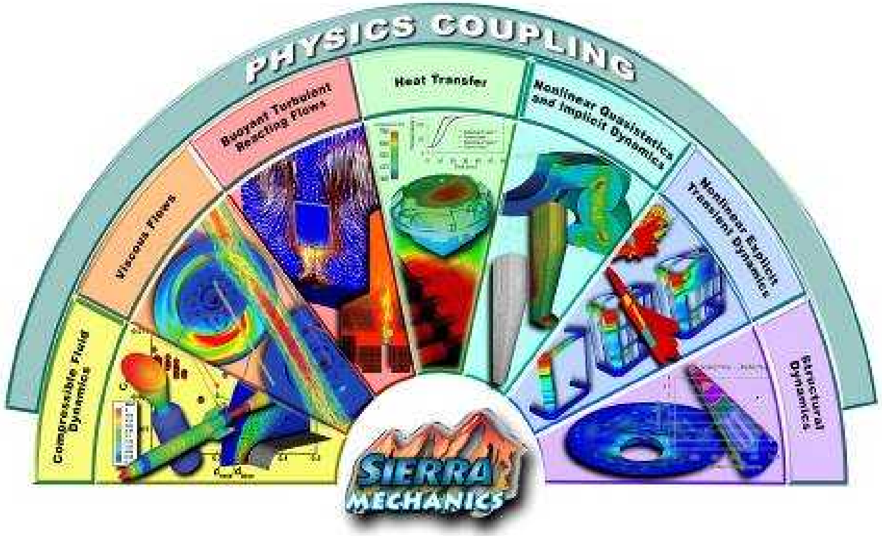
Sierra is the engineering mechanics simulation code supporting the NW mission, as well as other customers

- **Distinguishing strengths**
  - “Application aware” development
  - Scalable
  - SQA and V&V
  - Multiple scales
  - Coupling

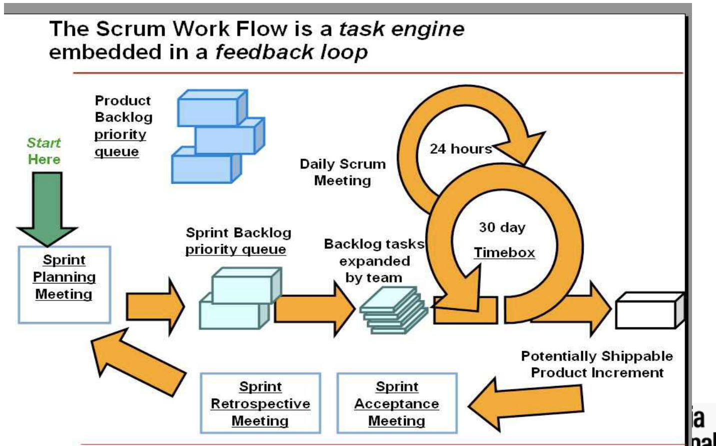


- **Explicit tie to SNL workflow, including**
  - Geometry and meshing
  - Visualization
  - Design and optimization

- **“Partner” applications include**
  - CTH and ALEGRA for shock physics simulations
  - RAMSES suite for radiation effects, electrical and electronics simulations

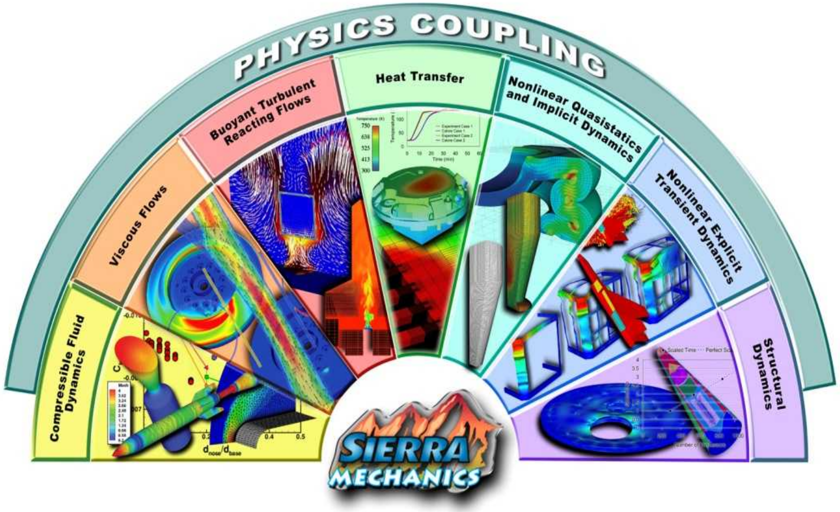
Sierra and Agile Software Development

- **All Sierra software development is done as "Agile Scrum Teams"**
  - SolidMechanics/StructuralDynamics
  - Thermal/Fluid
  - Toolkit/Framework
  - Infrastructure
- **Planning, retrospective and implementation is done within a *three* week development cycle**
- **Advantages:**
  - Quick adjustments to changing needs and new knowledge
  - Team ownership of the "product"
  - Team knowledge of the entire code base
  - Highly cooperative environment



There are three facets to the current code capability & consolidation efforts

- **Thermal/Fluids Consolidation**
  - Compressible Flow
  - Thermal Response
  - Multiphase
  - Turbulent Reacting Flow
- **Solid Mechanics Consolidation**
  - Explicit Transient Mechanics
  - Implicit Transient Mechanics
  - Quasistatics
  - Structural Dynamics
- **SIERRA Framework → SIERRA Toolkit**



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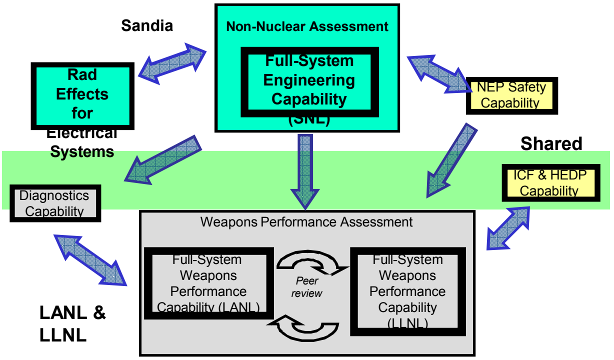
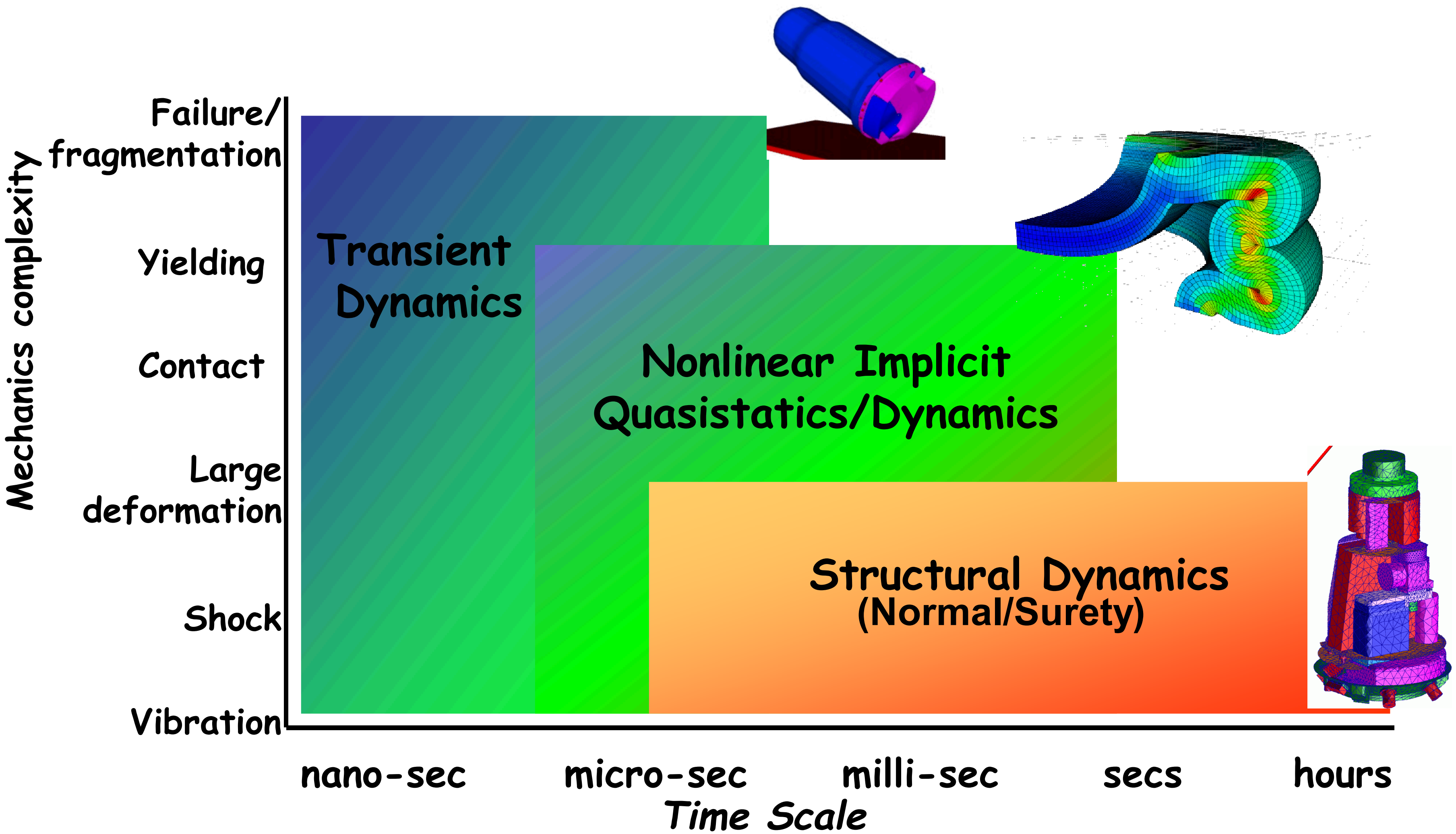
Code Consolidation is required for improved capabilities and technical “sustainability”



- **User Benefits:**
  - Flexibility in algorithms design
    - Implicit vs. explicit coupling
    - Added robustness and faster convergence
  - Tightly-coupled capabilities in “one” code
    - Consistent syntax
  - Faster response to user needs
    - Agile programming teams, simplified distribution

- **Development Benefits:**
  - Capabilities need not be duplicated
    - Though under one Framework, implementation details of adaptivity, error estimation, load balancing, solution control, etc., are duplicated in each code
  - Agile programming teams.
    - Previously: 1 or 2 developers per code
    - Now: core team contributing to all application areas
    - Core team is growing as more developers gain experience
  - Simplified distribution
    - Reduced inter-code dependence make releasing and shipping code easier
  - Increased collaboration between different groups

Sierra includes solid mechanics and structural dynamics capabilities



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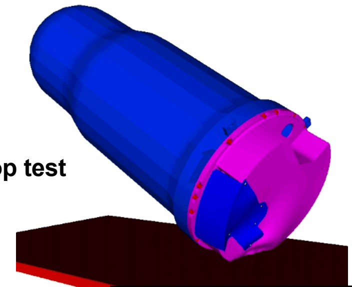
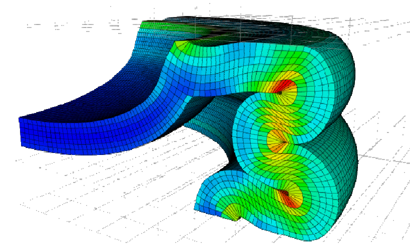
Explicit transient dynamics and implicit quasi-statics and dynamics capabilities

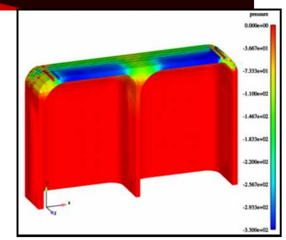
- **Fully Three-Dimensional**
- **Finite Elements and Particles**
  - Hex and Nodal Based Tets
  - Shell and Beams
  - SPH and Mass particles
- **Material models: 50+, including energy-dependent materials**
- **Explicit contact: Massively parallel, momentum balance, accurate friction response**
- **Multi-length Scale**
- **Boundary conditions:**
  - Kinematic and Force
  - Specialized: cavity expansion, silent BC
  - CONWEP integration (Analytic Blast Pressure Loads)
- **Explicit Failure modeling:**
  - Material failure/element death
  - Cohesive zones (elements, contact surfaces)
  - Phenomenological models (spot weld, line weld)
  - Automatic remeshing using Nodal Based Tets
  - X-FEM (pervasive failure modeling)
- **Quasi-static failure modeling**



W80 drop test



Large deformation/contact



Coupled Thermal/QS/Dynamic

- **Provides scalable parallel solvers for highly nonlinear problems**
  - Contact
  - Nonlinear material response
  - Large deformation
- **Utilizes services provided by the Sierra Framework/Toolkit to enable**
  - Coupled physics
  - Multi-length scale modeling techniques
  - Preloading

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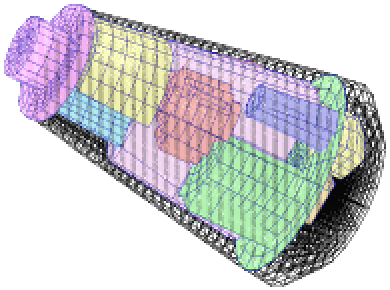
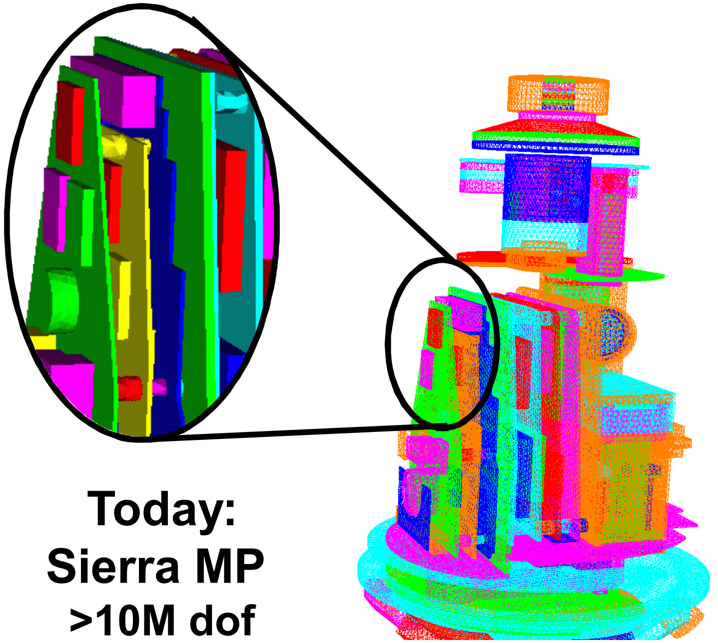
Structural Dynamics

- **Predicts the response of a system under dynamic conditions.**
  - Stresses (particularly in the operating regime)
  - Fatigue
  - Energy dissipation in joints
- **Efficient for very large problems**
  - Many millions of coupled equations
  - Serial, direct matrix solutions scale to order N^3
  - Parallel, iterative solvers are typically more complex, but scale as O(N)
    - FETI
    - CLIP, CLOP Solvers (Sandia)
- **Structural Acoustics**
- **Inverse Problem Capability underdevelopment**

Recent Past:
NASTRAN
MC2912
30,000 dof

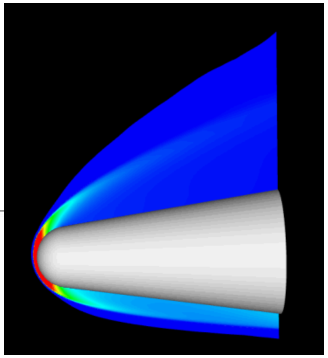


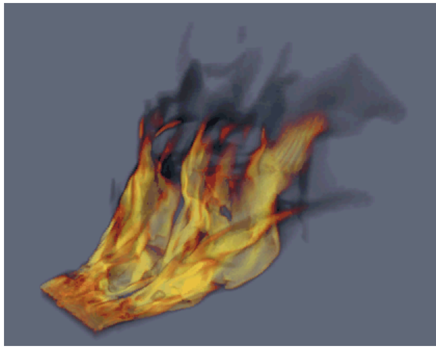


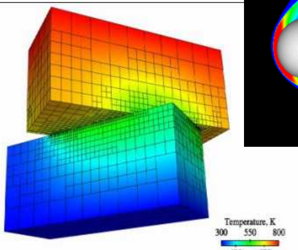
Today:
Sierra MP
>10M dof

Computational Thermal & Fluid Mechanics

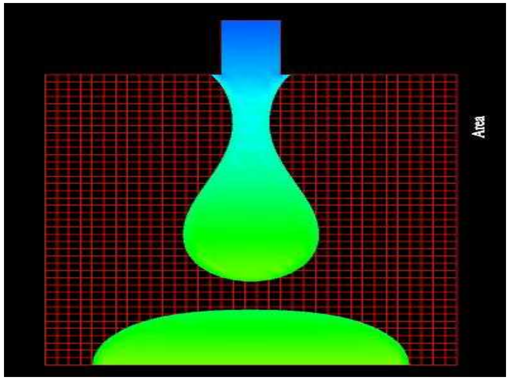
- Thermal – Heat Transfer, Enclosure Radiation and Chemistry
  - Dynamic enclosures
  - Element birth death
  - Contact
- Aero – Compressible Fluid Mechanic
  - Subsonic through hypersonic
  - Laminar and turbulent
  - Unstructured mesh



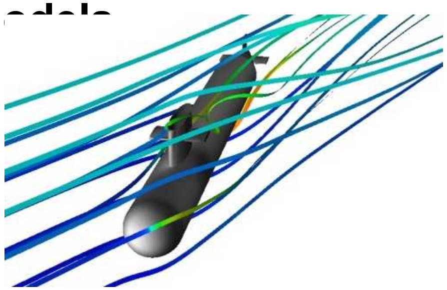




- Multiphase – Non-Newtonian, Multi-physics, and Free Surface Flows
  - Complex material response
  - Level sets for surface tracking
  - Flexible coupling schemes



- Fire/Combustion – Low Speed, Variable Density, Chemically Reacting Flows
  - Eddy dissipation and mixture fraction reaction models
  - RANS and LES based turbulence models
  - Unstructured Mesh
  - Pressurization models



Sierra/Thermal Capabilities

- **Governing Equations**
  - 3D unsteady, energy equation
  - Volumetric heat sources
    - Chemistry - heat of reaction
    - Arbitrary Q(x,t)
    - Arbitrary Q(T)
    - $Q(\phi)$, ϕ = solution field
- **Solution Algorithm**
  - 2nd order GFEM scheme
  - Weighted residual form
  - Integration by parts
  - Stabilization for advection
  - 1st order: Forward Euler/Backward Euler
  - 2nd order: Adams-Bashforth/Crank-Nicolson
  - Automatic time stepping
- **Spatial Discretization**
  - Isoparametric elements
  - Super-parametric elements
- **Thermal Capabilities**
  - **Enclosure radiation**
  - **Banded wavelength enclosure radiation**
  - **Generalized contact**
  - **ChemEQ chemistry model (w/ activation & deactivation controls)**
  - **Local coordinate systems for anisotropic materials**
  - **Standard and gradient shells**
  - **Block toggling/skinning capabilities**
  - **Thermoelectric coupling**
  - **Bulk fluid element capability is nearly complete**
  - **Element death capability is underway (CDFEM approach)**
- **Boundary Conditions**
  - **Temperature, Specified Flux, Convective Flux, Radiative**
  - **Flux, code specified or from transfers**

Sierra/FluidDynamics Aero Capability

- **Governing Equations**
  - 2D/3D compressible RANS
  - Ideal gas and non-equilibrium chemistry
- **Solution Algorithm**
  - Fully-implicit, fully-coupled, stabilized finite element formulation (SUPG)
  - Linear Lagrange basis: second order
  - First and second order time integration
  - Fixed or auto time step size selection
  - H-adaptivity
- **Viscosity Models**
  - Sutherland's viscosity law
  - Keyes' viscosity law
- **Turbulence**
  - **Spalart-Allmaras turbulence model**
  - **k-ω turbulence model**
  - **Menter's k-ω turbulence model**
- **Boundary conditions:**
  - **Supersonic inflow**
  - **Supersonic outflow**
  - **Subsonic inflow (reservoir)**
  - **Subsonic outflow (pressure)**
  - **Slip/symmetry**
  - **No slip isothermal wall**
  - **No slip adiabatic wall**
  - **Blowing wall, Coupled aerothermal heating**

Sierra/FluidDynamics Fire Capabilities

- **Solution Algorithm**
  - 2nd order CVFEM Scheme
  - Backward Euler and Steady solver; variety of predictors
- **Pressure Stabilization**
  - Second order and fourth order pressure stabilization
  - Time step and characteristic scaling
- **Coupling Strategy**
  - Fully-coupled scheme
  - Fully-segregated scheme
- **Property Evaluations**
  - Cantera along with standard Aria properties
- **Convection Operators**
  - Upwind, Geometric upwind and Central with automatic blending
- **Energy/Species**
  - Temperature form (heat conduction) and static Enthalpy
  - Arbitrary subindex-ed mass fraction (EDC combustion) and mixture fraction transport
  - Non-unity laminar transport with energy due to mass transport and correctional terms for appropriate behavior for j_{jk}
- **Turbulence**
  - LES Ksgs, TFNS, k-ϖ and k-ε
  - Iso-tropic eddy viscosity closure
  - Gradient diffusion closure for scalars (h, Y_k, Z_k)
- **Boundary Conditions**
  - Inflow, Open (dynP), Symmetry, Wall Function

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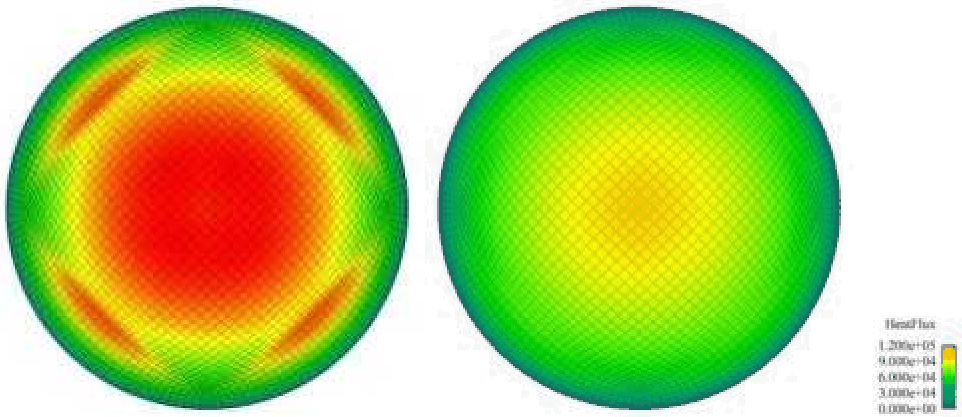
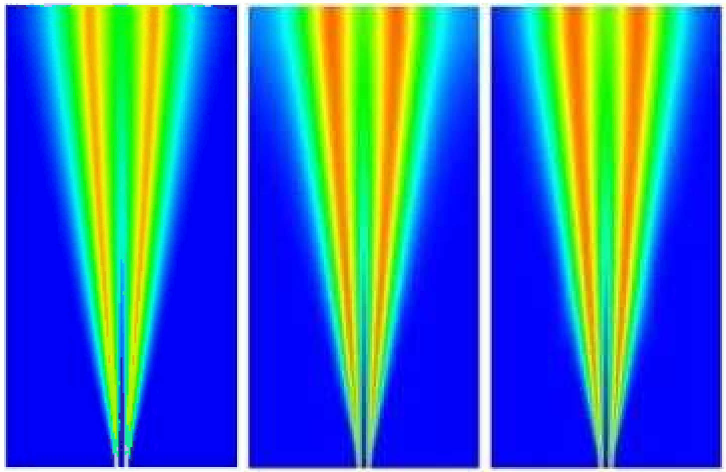
This shows three examples of increased capabilities resulting from consolidation

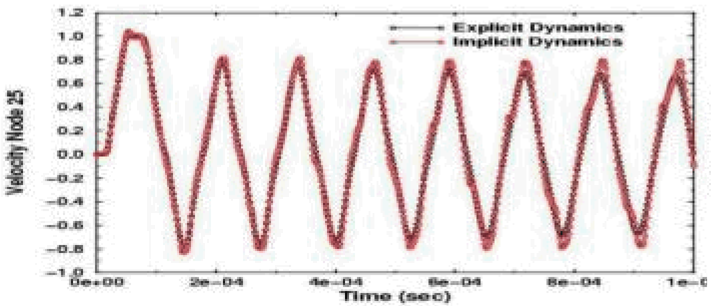


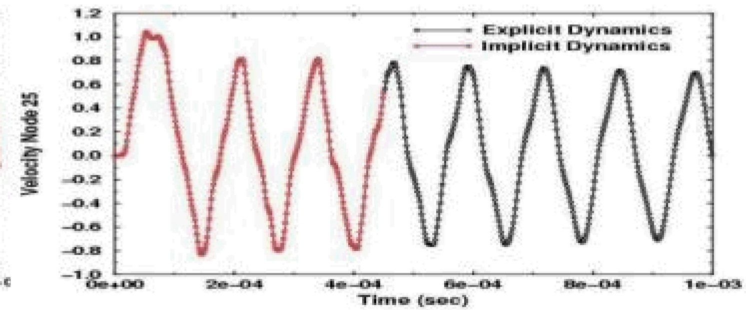
Sandia's SUPG algorithm for hypersonic flow almost eliminates grid dependencies



Fully Segregated | **Fully Implicit** | **Partial Segregated**

New couplings for low speed flow improve accuracy





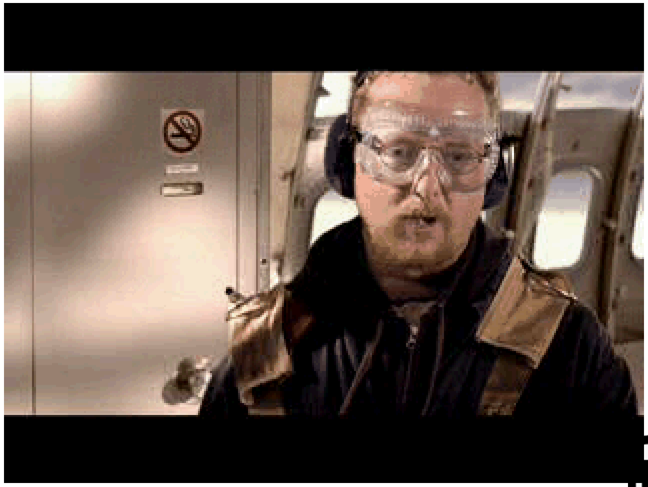
Implicit and explicit transient dynamics calculations can be run separately (left) or with on the fly switching (right)

The Sierra Toolkit is the basis for consolidation, sustainability and external engagement

- **SIERRA Toolkit**
  - Goals
    - Make framework services available as separate tools in a toolkit.
    - Modernize software design and simplify APIs
    - Encapsulate hybrid mpi/threads parallel model at the algorithm support level.
    - Open source: available via Trilinos
  - Benefits
    - Improve agility and robustness
    - Broader application space
    - Improve coupling, especially external to Sierra
    - Prepare for exascale

- **Sierra "engagement" strategy**
  - Layer 1 – open-source toolkit and "demo app"
  - Layer 2 – EAR99 application
  - Layer 3 – EC and ITAR

- **SIERRA Framework Refactor**
  - Minimize impact on current applications: incremental refactor instead of complete rewrite -> like building a plane in the air.
  - Phase 1: refactor the current framework to reflect the smaller API and some of the main domain model concepts from the initial toolkit mesh module.
  - Phase 2: pick a current SIERRA application module and refactor it completely to use the SIERRA Toolkit – use as a discovery effort.
  - Phase 3: Based on outcome from phase 2, develop final refactor path for the primary application modules.



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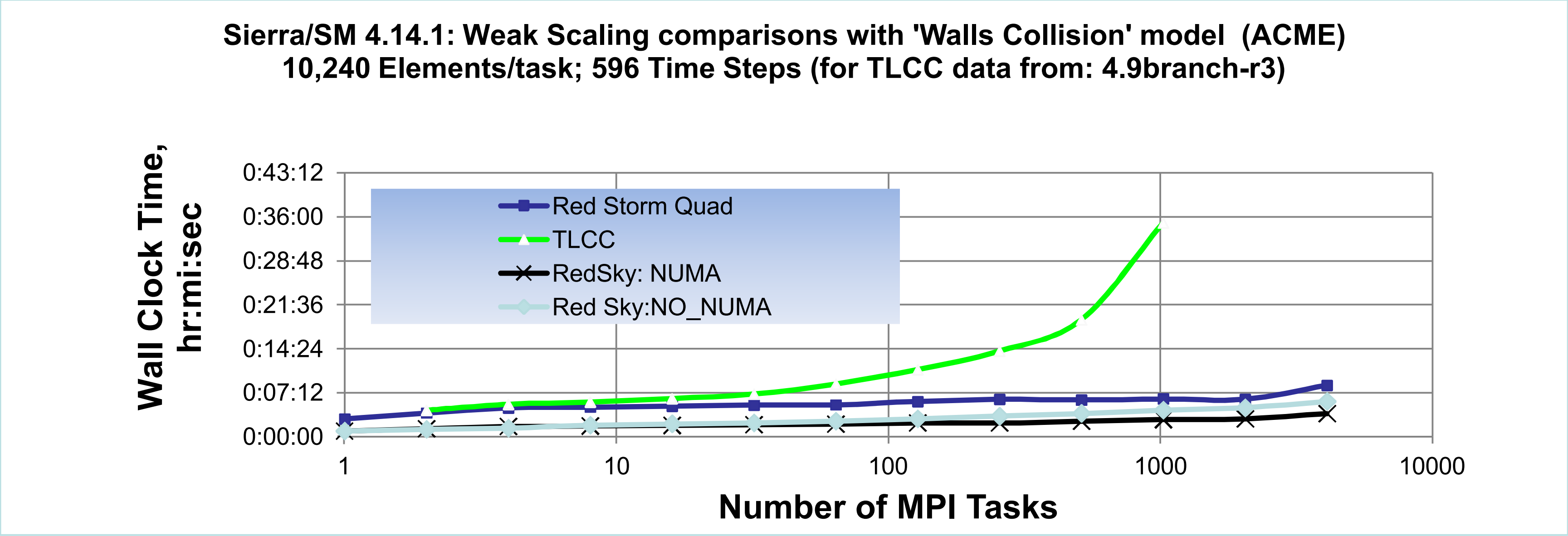
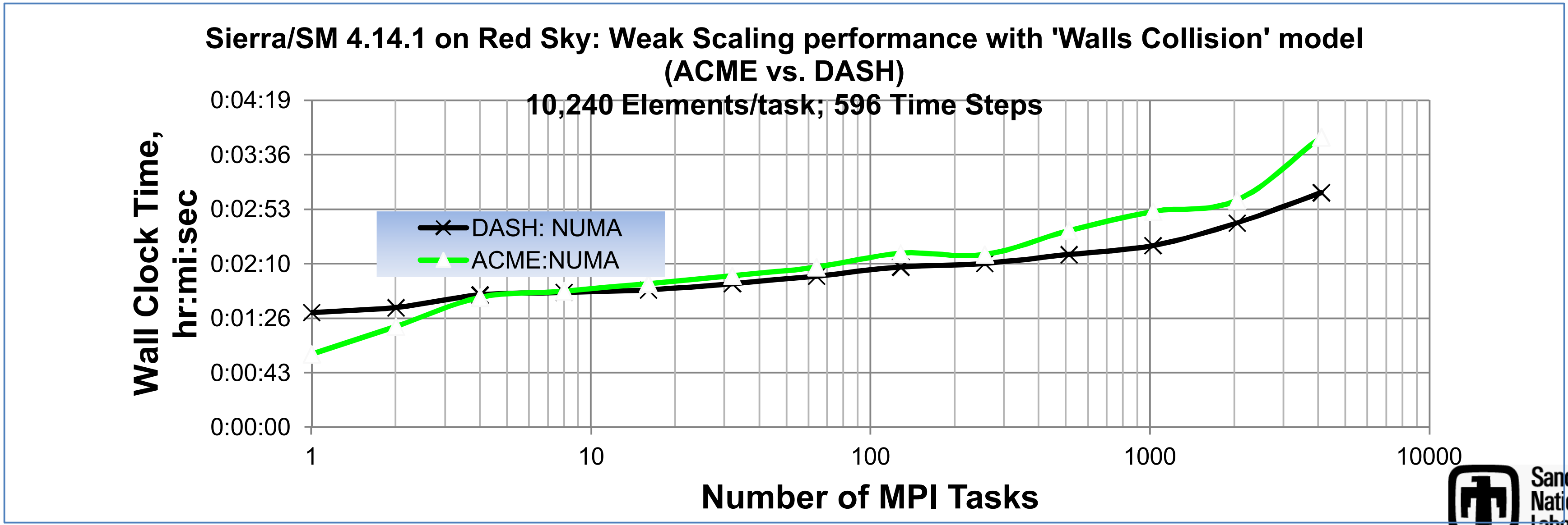
SIERRA/SM(explicit) Scaling on Red Sky





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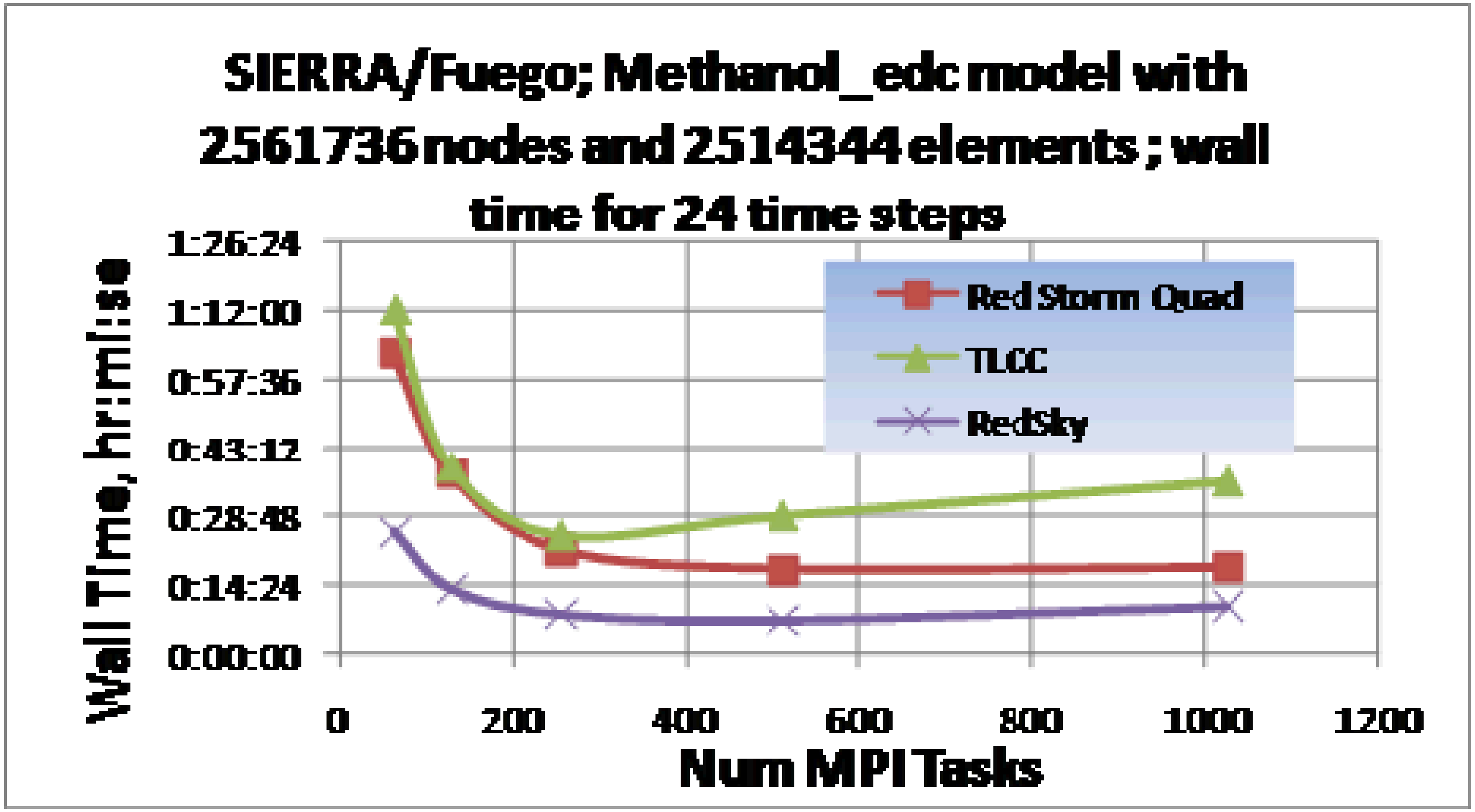
SIERRA/FluidDynamics (Fire) Scaling



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Sierra will incorporate the concept of "intrinsic V&V"

- **Goals**
  - V&V/UQ is pervasive in our simulation work; it is not an "add-on" or an "outer layer"
  - We provide analysts with all the relevant V&V information for their simulations
- **Examples of current intrinsic V&V capabilities**
  - Solution verification via uniform mesh refinement (via Encore): estimate errors, rates of convergence
  - Parameter sensitivities (limited application coverage): provide first-order sensitivities of simulation output to parameters (e.g. eigenvalue/eigenvector sensitivities to material parameters)
  - SIERRA Feature Coverage Tool (FCT) for code verification (next slides)

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Sierra meets rigorous SQA, verification and acceptance testing standards

- Sierra teams develop code using scrum-based (agile) programming methodology
- Sierra implements ASC/SQA practices
- Sierra will provide metrics on code and feature coverage for tests and provide evidence for code verification
- Example of SD/SM verification suite scale
  - Regression test suite (RTS) ~8000 is used to test code check-ins for bugs
  - Verification test suite (VTS) ~600 is used to verify code's ability to solve problems with known/expected solutions and/or expected rates of convergence
  - Example test suite (ETS) ~50 is used demonstrate code features and capability usage guidelines
  - Performance test suite (PTS)~50 is used to test performance of code's implementation of various algorithms and to benchmark performance vs. other codes
  - Acceptance test suites (ATS) ~70 are used to test code's acceptance for an application space

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Each Sierra module has a verification test suite

Sierra Capabilities (subset)

	Application									Verfication Test Suite																																												
										1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44
PDE terms																																																					
Conduction (diffusion term)	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
Capacitance (transient term)	X	X	X	X	X	X	X	X	X	X			X			X	X	X	X				X									X	X				X	X	X							X	X	X	X	X	X	X	X
Src (source term)	X	X									X	X	X								X	X		X	X				X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X						
EnclRad	X	X	X	X	X	X	X	X	X											X																																	
CM (chemistry source term)													X										X																														
Thermal Conductivity																																																					
k0 (constant conductivity)	X	X	X	X	X	X	X	X	X				X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X			X	X	X	X
k1 (tabular T-dependant)	X	X	X	X	X	X	X	X	X																			X																				X	X				
k2 (user subroutine T-dependant, mostly)		X				X	X	X		X	X	X																																									
k3 (defined variable)																																																					
k4 (anisotropic constant)	X	X		X			X		X																																									X	X	X	
k5 (anisotropic tabular T-dependant)	X	X	X	X					X																																												
Heat capacity																																																					
Cp0 (constant)	X	X	X	X	X	X	X	X	X				X					X	X				X									X	X				X	X	X							X	X			X	X	X	X
Cp1 (tabular T-dependant)	X	X	X	X	X	X	X	X	X							X	X																																X	X				
Cp2 (user subroutine T-dependent)		X				X		X		X																																											
Cp3 (user variable)																																																					
Density																																																					
D0 (constant)	X	X	X	X	X	X	X	X	X	X			X			X	X	X	X				X									X	X				X	X	X							X	X	X	X	X	X	X	X
D1 (tabular T-dependent)			X	X		X		X	X																																												
D2 (user subroutine T-dependent)		X																																																			
D3 (user variable)																																																					
D4 (volume dependant)																																																					
Source terms																																																					
G0 (constant)	X	X																			X	X							X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X						
G1t (tabular, time varing)	X																																																			
G1T (tabular, temp varing)																																																					
G2 (user subroutine, time or temp varing)		X									X	X	X												X	X																												
G3 (user variable)																																																					
Temperature boundary conditions																																																					
T-0 (constant)	X				X	X	X				X	X	X	X	X					X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X						
T-1t (tabular, time dependent)					X																																															
T-2 (user subroutine)						X	X						X																																							
Flux boundary conditions																																																					
Q-0 (constant)																	X	X		X	X							X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		X	
Q-1t (tabular, time dependant)			X																																																		
Q-1T (tabular, temp dependant)																																																					
Q-2 (user subroutine)				X					X	X						X	X																																			X		
Convective boundary conditions																																																					
h-0 (constant)	X	X	X	X	X	X															X	X							X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X						
h-1t (tabular, time dependent)			X																																																		
h-1T (tabular, temp dependent)																																																					
h-2 (user subroutine)																																																					
Tref-0 (constant ref temp)	X	X	X	X	X	X															X	X							X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X						
Tref-1t (tabular, time dependent, ref temp)	X																																																			
Tref-1T tabular, temp depentdent, ref temp)																																																					
Tref-2 (user subroutine, ref temp)																																																					
Tref-B (bulk fluid element)			X	X																																																	
Radiation boundary conditions																																																					
e-0 (constant emissity)	X	X	X	X																																																	X
e-1 (tabular, T-dependent)			X	X																																																	
e-2 (user subroutine, T dependent)		X																																																			
Trad-0 (constant radiation temperature)	X	X	X	X																																																	X
Trad-1t (tabular, time dependent rad temp)	X																																																			

Sierra will continue to invest in new capabilities

- Nonlinear stress response (w/ multi-level solvers)
- Interface problems (contact)
- Large deformations (automatic remeshing, particle methods)
- Failure Modeling
  - Element death
  - Element to Particle
  - Dynamic Cohesive Zone
  - X-FEM
- Multi-Scale Modeling:
  - RVE (representative volume element)
  - Embedded Finite Element models
  - Time
- Performance
  - Solvers
  - Contact Algorithms
  - Element calculations
- Nonlinear Structural Acoustics
- Energy Dissipation
- Time and Frequency Domain vibrations

- Unified FEM algorithms for high speed compressible flows, fire applications, and porous flow with deformable media applications
  - Improved accuracy via analytic enrichment for steep gradients
- Improved thermal contact and enclosure radiation
- Improved finite rate chemistry and fluid/thermal ablation coupling for re-entry
- Improved Fluid (Aero)-Structure interaction
- Couplings to: Thermal, Solid, Fluid, Shock Hydro
  - Including large deformation Fire-Thermal-Structural coupling
- Intrinsic V&V
  - Testing and verification
  - Uncertainty quantification
- Support
  - User support
  - Documentation and training
  - Usability and workflow
- Continued development of the toolkit
  - MPP capabilities and advanced architectures
- Inverse problems and design

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